Simulation of the 2D Ising model - Metropolis algorithm

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1 The 2D Ising model

Imagine a LxL square lattice where each site j is occupied by a spin s_j that can take the value $+1$ or -1. One particular combination of $N = L^2$ spins, $\{s_1, s_2, ..., s_N\} = \{\mathbf{s}_i\} = i$, defines one configuration/state (all possible states of a system with N sites is 2^N) of the system and it corresponds to a specific amount of energy according to the usual Hamiltonian with nearest neighbor interactions and zero external magnetic field,

$$\mathcal{H}_i = E_i = -J \sum_{<j,k>} s_j s_k$$

Where J is a positive constant that defines the energy scale of the problem and favors parallel alignment between two neighboring spins ($-J$). In case two neighboring spins are anti-parallel to each other, the energy of interaction is $+J$. The magnetization (per spin) of the system in state i is given by,

$$m_i = \frac{1}{N} \sum_j s_j$$

At a given temperature, T, our system has both energetic contributions to the free energy as well as entropic ones. Remember from class,

$$A = \langle E \rangle - T\langle S \rangle \xrightarrow{?} E - TS$$

At very low T all spins are aligned and we have an energetically favorable situation,

$$\langle E \rangle = -2NJ$$

Entropy of a state where every spin points upwards?

It is interesting to look at those states that dominate for a given T. Find that perfect sweet spot between energy and entropy. Apparently for low temperatures there is scarcity of thermal energy available and spins orient upwards

(or downwards) giving rise to the ferromagnetic phase $m = +1$. On the other hand at high temperatures we have a 50:50 mixture of spins namely a paramagnetic phase where $m = 0$.

The question is: What kind of phase transition do we have? 1st order? 2nd order? Perhaps no transition at all? How does the $\langle m \rangle$ vs T diagram looks like?

2 Direct calculation

What is the simplest possible approach to calculating thermodynamic variables?

A few naive ideas and why we will need a more sophisticated algorithm like Metropolis. In principal we could just start going through every each one configuration of the system (How many?), calculate its energy

$$E_i = -J \sum_{\langle j,k \rangle} s_j s_k$$

Calculate the unnormalized probability based on the Boltzmann distribution,

$$p_i = \exp\left(\frac{-E_i}{k_B T}\right)$$

After that we would calculate the partition function,

$$\mathcal{Q} = \sum_i p_i = \sum_i \exp\left(\frac{-E_i}{k_B T}\right)$$

Then we would be able to calculate thermodynamic properties as well as the magnetization at thermal equilibrium for each possible value of T,

$$\langle E \rangle = \frac{\sum_i p_i E_i}{\mathcal{Q}}$$

$$\langle m \rangle = \frac{\sum_i p_i m_i}{\mathcal{Q}}$$

Why can't we just do that? Just like we did in the 1d case in class. Turns out we can't find analytical expression for the sum in most models. Therefore we need approximate solutions or computer simulations.

3 Will this work?

Think of a 5x5 square lattice with 25 spins. The total number of states is,

$$2^{25} \approx 10^7$$

Technically we can write all the possible states down and by calculating the energy of each state we can evaluate the partition function, the energy, the

magnetization, the heat capacity etc. Problem: TAKES FOREVER. For a lattice of 10x10 the number of states is

$$2^{100} \approx 10^{30}$$

That means that we can't use all of the states of the system in order to calculate thermodynamic properties. We have no choice but to pick a subset M of all the possible states. The question boils down to HOW DO WE GENERATE M EFFECTIVELY?

4 Monte Carlo - Statistical Sampling

It is an old mathematical idea called statistical sampling where we generate configurations randomly (thus the casino inspired name of the method). All states have an equally likely chance of getting picked. Take for example a tiny system of 10x10 . The total number of possible states is $2^{100} \approx 10^{30}$. Since we are limited by computational power we will rely on ,

$$M = 10^6$$

randomly generated states. The probability of choosing each one of the 10^{30} states is the same,

$$\pi_i = \frac{1}{10^{30}}, \forall i \in \{1, 2, ..., 10^{30}\}$$

Let's see what could go wrong with that procedure. Imagine we simulate a very cold system where $k_B T$ is very small. Only very ordered states are gonna be thermally accessible and will have significant contribution in the calculation of the partition function,

$$\mathcal{Q} = \sum_{\text{high order states}} \exp\left(\frac{-E_i}{k_B T}\right) + \sum_{\text{rest of states}} \exp\left(\frac{-E_i}{k_B T}\right)$$

Same for averages,

$$\langle E \rangle = \sum_{\text{high order states}} P_i E_i + \sum_{\text{rest of states}} P_i E_i$$

The second term in both equations is going to be very small because the Boltzmann weights are gonna be tiny (there is not enough thermal energy to access them),

$$\sum_{\text{rest of states}} E_i P_i = \text{tiny}$$

So you see the problem here. Both unimportant and important states have equal probability, π_i, of being chosen and so we spend precious computational time sampling states with little to no contribution to our sums. That is poor sampling. Why would you even spend time calculating the energy of a very

disordered state since there is not enough thermal energy to get there and thus has a probability of zero. The opposite is true for high k_BT where entropy dominates and calculating the energy of very ordered states is a waste of time. Need a more intelligent method than generating samples with equal probability.

5 Metropolis algorithm

This is why the Metropolis algorithm was born in Los Alamos in 1953. Now we start from a random spin configuration and transition gradually to the "important" states. The basic quantity is the **transition probability**, $P(X \to Y)$, from one state to another and needs to satisfy the so-called **detailed balance**. This is the heart of the simulation and is actually a chemistry idea. Imagine the following reaction,

$$\mathrm{X} \underset{k_{Y\to X}}{\overset{k_{X\to Y}}{\rightleftharpoons}} \mathrm{Y}$$

At equilibrium we have,

$$k_{X\to Y}[X] = k_{Y\to X}[Y]$$

Similarly we can think of a detailed balance between two states X and Y instead of reactants,

$$P(X \to Y)P(X) = P(Y \to X)P(Y)$$

or,

$$\frac{P(X \to Y)}{P(Y \to X)} = \frac{P(Y)}{P(X)}$$

If you think about it, the probability that our system will go from X to Y is simply the product of two factors: How probable it is that our system will propose that move and how probable it is that our algorithm will accept the move. Mathematically that means,

$$P(X \to Y) = g_{prop}(X \to Y)A(X \to Y)$$

But in our case the probability that we propose one move will be the same with the probability of proposing the reversible move,

$$g_{prop}(X \to Y) = g_{prop}(Y \to X)$$

Starting from an initial lattice we propose a single spin flip every time. The probability of the opposite step is going to be the same. Lastly, the probabilities of each state are chosen form the Boltzmann distribution so,

$$\frac{P(X \to Y)}{P(Y \to X)} = \exp\left(-\beta(E_Y - E_X)\right)$$

So that leaves us with the following expression,

$$\frac{A(X \to Y)}{A(Y \to X)} = \exp\left(-\beta(E_Y - E_X)\right)$$

This is the final part of the algorithm where you choose the next state based on the energy difference,

$$A(X \to Y) = \begin{cases} \exp\left(-\beta(E_Y - E_X)\right), & E_Y > E_X \\ 1, & E_Y < E_X \end{cases}$$

Basically you pick a random spin in the lattice, flip it, measure the energy difference. If the new energy is lower you accept the move with 100% probability. If the new energy is higher then you accept the move with probability of $\exp\left(-\beta(E_Y - E_X)\right)$x100%. This process will eventually generate a sequence of spin configurations that are guaranteed to reach the Boltzmann distribution.

6 Results

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